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Computing Novel Multiplicative Zagreb Connection Indices of Metal-Organic Networks (MONs)

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Abstract

Topological index (TI) is a mathematical formula which represents a (molecular) network using graph isomorphism. TI also predicts the toxicological, structural, biological and physicochemical properties of a chemical compound. Metal-organic network (MON) is a recently developed chemical compound having versatile applications in heterogeneous catalysis, environmental hazard, super- capacitors, absorption analysis, energy and gas storage device, sensing, and the assessment of several chemicals. MON consists of vertices (or metal ions) and edges between vertices (or linkers) that provides a huge surface area, excellent chemical stability, unique morphology, octahedral cluster, and a large pore volume. At present, zinc based MONs are also used in biomedical applications such as cancer imaging, drug delivery, and biosensing. In this paper, we initially define the fourth and fifth multiplicative Zagreb connection indices (ZCIs). We also compute the first, second, third, fourth and fifth multiplicative ZCIs of two different zinc based MONs, namely zinc oxide network (R) and zinc silicate network (S).

Keywords: connection number, metal-organic networks, multiplicative Zagreb indices

Introduction

Metal-organic network (MON) is the most popular chemical compound dealings with metal-ion and organic-ligand. This network has a large diameter, intensive area, and giant pore volume. A variety of MONs have been discovered in modern chemistry. Zinc based MONs can be used to discover luminescent thermometers, see [\[1\]](#page-20-0). Luminescent sensors are also used in the electron rich T-conjugated fluorescent ligand with the help of Zn based MON, see $[2]$. Moreover, MONs are widely used in the

assessment of chemicals, energy and gas storage devices, adsorption analysis, toxicology, biomedical application, separation of several gases, biocompatibility, environmental hazards and heterogeneous catalysis. For this reason, the mechanical properties and physical stability of these MONs have become a topic of interest among scientists and researchers.

In non-linear optically processes, active MON Zn^{2+} is averagely used as a connecting points to overcome devalued d-d transition in the visible regions. The bio-medical applications, toxicology, and bio-compatibilities are currently the suggested production procedures of Zn based MONs, see [\[3\]](#page-20-2). Eddaoudi et al. [\[4\]](#page-20-3) studied 16 highly crystalline compounds (IRMOF-1 to IRMOF-16) that are also known as the isoreticular series of MONs. The range of fixed and free diameters is 3.8 -19.1 A^0 and 12.8 -28.8 A^0 for IRMOF-1 to IRMOF-16. All IRMOFs have an ordinary topology $CaB_6(13)$ and appear according to the structure of IRMOF-1 such as Zn_4O tetrahedrons. Several IRMOFs such as IRMOFs-(8,10,12 and 16) have non-crystalline networks. For more information, we refer to [\[5-](#page-20-4)[7\]](#page-20-5).

MON also predicts some properties such as impregnating suitable active material [\[8\]](#page-20-6), grafting active groups [\[9\]](#page-20-7), biosensors enhancing selectivity $[10]$, post synthetic ligand $[11]$, changing organic ligands and ion exchange [12]. In his study, Lin et al. [\[13\]](#page-21-1) (2009) presented MONs related applications such as production-catalyst, photo-catalysis, sensing, electro-catalysis, and super-capacitors. MONs also have versatile applications such as the delivery of drugs [\[14\]](#page-21-2), adsorption [\[15\]](#page-21-3), storage of gases [\[16-](#page-21-4)19], catalysis for the separation and purification [\[20,](#page-22-0) [21\]](#page-22-1). Graph theory uncovered various numerical tools that are utilized in many sectors of science such as mathematical chemistry, pharmacology, pharmaceutical, computer science, drug discovery process, medicinal- and bio-chemistry. These numeric apparatuses depict the physicochemical properties of chemical materials liked flash point, tension, boiling point, partition coefficient, correlation coefficient, temperature, heat of formation and evaporation, see [\[22-](#page-22-2)[24\]](#page-22-3).

For the first time in the history of graph theory, Gutman and Trinajstić [\[25\]](#page-22-4) (1972) discussed degree based topological index (TI) to check the π electron energy of a chemical compound. At present, these TIs are

abundantly used in the study of QSAR/QSPR and the latest porous materials known as MONs. Awais et al. [\[26\]](#page-22-5) studied two different MONs, namely $MON_1(p)$ and $MON_2(p)$, where $p \ge 2$ with the help of generalized indices and their connection indices. Hong et al. [\[27\]](#page-22-6) used these MONs to identify chemical suitability among a few well-known degree based TIs. Recently, several authors also used the concept of MONs in the shape of line graphs to study some of their physical properties for different TIs. They also computed neighborhood and Mpolynomials for different TIs of MONs [\[28,](#page-22-7) [29,](#page-23-0) [30\]](#page-23-1). For more knowledge about MONs insight of TIs, see [\[31-](#page-23-2)[33\]](#page-23-3).

Tang et al. [\[34\]](#page-23-4) used the concept of connection number, defined by Gutman and Trinajstić in [\[25\]](#page-22-4) to compute the first Zagreb connection index (ZCI). They also computed modified first ZCI of the sub-division based operations on networks. At present, the TIs based on degree and connection number are abundantly used in four layer neural networks see [\[35\]](#page-23-5). Javaid et al. and Liu et al. [\[36,](#page-23-6) [37\]](#page-23-7) computed the TIs of rhombus silicate, rhombus oxide networks, and cellular neural networks. Javaid and Jung [\[38\]](#page-23-8) and Raheem et al. [\[39\]](#page-24-0) computed M-polynomial based TIs of silicate and oxide networks and two dimensional lattices of three layer single wall titania- nanotubes. Moreover, Zhao et al. [\[40\]](#page-24-1) computed reverse degree based TIs of zinc based MONs. Additionally, connection number (or leap degree) based TIs are used to classify different classes of networks, see [\[41-](#page-24-2)[47\]](#page-24-3).

In this paper, we define the novel multiplicative fourth and fifth ZCIs. We compute multiplicative first, second, third, fourth and fifth ZCIs of zinc oxide (IRMOF-10) and zinc silicate (IRMOF-14) networks. The structure of the given paper is as follows: Section II provides preliminaries**,** basic definitions, and partitions of MONs. Section III gives the main results of MONs, while Section IV is dedicated to the conclusion of this study.

2. Preliminaries

Let K be any connected simple graph. The cardinalities of the edge set $(|E(K)|)$ and vertex set $(|V(K)|)$ are equal to v and u, respectively. Let $d_K(m)$ is the simple degree and $\tau_K(m)$ is the connection number of any

vertex m. The average degree is denoted by $\overline{d_K}(m)$ and defined as . $d_{\kappa}(m)$ $\overline{d}_K(m) = \frac{\sum_{m \in V(K)} a_K}{m}$ *u m* $\overline{d}_K(m) = \frac{m \in V(K)}{m}$ *K* $\sum_{v \in V(K)} d_K(m)$. The computed value of the average degree of any graph holding order u and size v is $\frac{2v}{ }$. *u* $\frac{v}{x}$. The average connection number is $\overline{\tau_K}(m)$ and observed as $\overline{\tau_K}(m) = \frac{m\epsilon V(K)}{m}$. (m) $\frac{1}{\tau_K}(m) = \frac{\sum_{k=1}^{K} K_{k}}{K}$ *u m* $m) = \frac{m \in V(K)}{m}$ *K* $\sum_{e \in V(I)}$ τ $\tau_K(m) = \frac{m\epsilon V(K)}{m}$. The computed value of average connection number of each graph having order u and size v is $\frac{1}{2}(K) - 2\nu$. *u* $M_1(K)$ – 2 ν . For more notations, terminologies, degree and connection number of a vertex, we suggest to see [\[48,](#page-24-4) [49\]](#page-24-4).

Definition 2.1. For a (molecular) network K, the first, second and third Zagreb indices are defined as

(a)
$$
M_1(K) = \sum_{n \in V(K)} [d_K(n)]^2 = \sum_{mn \in E(K)} [d_K(m) + d_K(n)],
$$

(b)
$$
M_2(K) = \sum_{mn \in E(K)} [d_K(m) \times d_K(n)],
$$

(c)
$$
M_2(K) = \sum_{mn \in E(K)} [d_K(m) \times d_K(n)],
$$

(c)
$$
M_3(K) = \sum_{n \in V(K)} [d_K(n)]^3 = \sum_{mn \in E(K)} [d_K^2(m) + d_K^2(n)].
$$

Gutman & Trinajstić [\[25\]](#page-22-4), Gutman et al. [\[50\]](#page-25-0), and Furtula & Gutman [\[51\]](#page-25-1) defined these degree based TIs to check the feasibility and chemical ability of several (molecular) networks such as correlation coefficient, ZEisomerism, molecular weight, entropy, acentric factor, heat capacity, density, volume, critical temperature, boiling point, acentric factor and entropy. For more properties, see [\[52,](#page-25-2) [53\]](#page-25-3).

Definition 2.2 [\[54\]](#page-25-4). For a (molecular) network K, the first and second multiplicative Zagreb indices are defined as follows:

(a)
$$
MZ_1(K) = \prod_{n \in V(K)} [d_K(n)]^2,
$$

(b)
$$
MZ_2(K) = \prod_{mn \in E(K)} [d_K(m) \times d_K(n)].
$$

Definition 2.3 [\[55\]](#page-25-5) For a (molecular) network K, the first multiplicative Zagreb index is also defined as follows:

$$
MZ_1(K) = \prod_{mn \in E(K)} \left[d_K(m) + d_K(n) \right].
$$

Definition 2.4. For a (molecular) network K, the first Zagreb connection index, second Zagreb connection index and modified first Zagreb connection index are defined as follows:

(a)
$$
ZC_1(K) = \sum_{n \in V(K)} [d_K(n)]^2,
$$

(b)
$$
ZC_2(K) = \sum_{mn \in E(K)} [\tau_K(m) \times \tau_K(n)],
$$

(c)
$$
Z C_1^*(K) = \sum_{n \in V(K)} [d_K(n) \times \tau_K(n)] = \sum_{mn \in E(K)} [\tau_K(m) + \tau_K(n)].
$$

In 2018, Ali and Trinajstić [\[56\]](#page-25-6) redefined these connection number based ZIs. They checked these TIs on the thirteen physicochemical properties of octane isomers. They also reported that ZC_1^* – index is more correlated among the others novel/old TIs.

Definition 2.5. For a (molecular) network K, the first, second and third multiplicative Zagreb connection indices are defined as follows:

(a)
$$
MZC_1(K) = \prod_{n \in V(K)} [\tau_K(n)]^2
$$
,

(b)
$$
MZC_2(K) = \prod_{mn \in E(K)} [\tau_K(m) \times \tau_K(n)],
$$

(c)
$$
MZC_3(K) = \prod_{n \in V(K)} [d_K(n) \times \tau_K(n)].
$$

Haoer et al. [\[57\]](#page-25-7) defined these connection based multiplicative Zagreb indices. They used these multiplicative indices the same as multiplicative leap Zagreb indices.

Definition 2.6. For a (molecular) network K, the fourth and fifth multiplicative Zagreb connection indices are defined as follows:

(a)
$$
MZC_4(K) = \prod_{mn \in E(K)} [\tau_K(m) + \tau_K(n)],
$$

(b)
$$
MZC_{5}(K) = \prod_{n \in V(K)} [d_{K}(n) + \tau_{K}(n)].
$$

Definition 2.7. Zinc Oxide Network (ZNOX(p)): Zinc oxide (ZnO) is a chemical compound which is insoluble in water. ZnO has a strong tendency for self organized growth. Also, the growth morphology of the ZnO (nanorings, nanobelts, nanosprings, nanowires, nanocages and nanocombs) is affected by the geometrical shape of the substrate. For this reason, ZnO is suitable for short wavelength optoelectronic applications. ZnO is also an inorganic compound. It has boiling point of 2360° C and density of 5.61 $g/c m³$. This unique material directly produces wide band gap $(\sim 3.4eV)$ ceramic n-tube semiconductors. Its hardness and thermal properties such as specific heat, Debye temperature and thermal conductivity, are dependent upon elastic coefficients of ZnO. ZnO has three acoustic phonon bands, one is longitudinal and the remaining two are transverse. The fact that ZnO has ionic bonding. The three coefficients of the piezoelectric tensors are d_{15} , d_{31} and d_{33} having values of -10, -5, and 12×10^{-2} mV^{-1} , respectively. ZnO is often applied in the production of glazes, rubber, the pigment in white paint, and photoconductive surfaces. $Zn_4O(BPDC)$ ₃ is also written as IRMOF-10, it is a three dimensional cubic networks having a pore size of $16.7/20.2$ A^0 in diameter, see [\[58\]](#page-25-8).

The MON of zinc oxide of dimension 3 is presented in Figure 1.

Figure 1. Metal organic network $(ZNOX(p) \cong R)$

Let $R \approx ZNOX(p)$ be the zinc oxide related metal-organic network of dimension p in the plane, see Figure 1. We take partitions of the network *R* with the help of vertex set $V(R)$ and edge set $E(R)$. We see that every vertex having a degree and connection number sets are $\{2,3,4\}$ and $\{2,3,4,5,8\}$ respectively. We have $V_1 = \{n \in V(R) | d_n = 2\}$, $V_2 = \{n \in V$ (R) | $d_n = 3$ } and $V_3 = \{n \in V(R) | d_n = 4\}$, where $|V_1| = 42p + 30$, $|V_2|$ $= 26p + 14$ and $|V_3| = 2p + 2$. So, $|V(R)| = |V_1| + |V_2| + |V_3| = 70p +$ 46. The partition of vertices with respect to connection number are $V_1 =$ $\{n \in V(R)|, \tau_n = 2\}, V_2 = \{n \in V(R)|, \tau_n = 3\}, V_3 = \{n \in V(R)| \tau_n = 3\}$ 4}, $V_4 = \{ n \in V(R) | \tau_n = 5 \}$ and $V_5 = \{ n \in V(R) | \tau_n = 8 \}$, where $|V_1| =$ $2p+6$, $|V_2| = 28p+20$, $|V_3| = 30p+10$, $|V_4| = 8p+8$ and $|V_5| = 2p+2$. So, $|V(R)| = |V_1| + |V_2| + |V_3| + |V_4| + |V_5| = 70p + 46$. Now, the partition of vertices with respect to degrees and connection numbers are $V_1 = V_d$, $V_{2,2}$ ={n \in V (*R*)| d_n = 2, τ_n = 2}, $V_2 = V_{2,3}$ ={n \in V (*R*)| d_n = 2, τ_n = 3 $\{y_1, y_2 = V_{2,4} = \{n \in V(R) | d_n = 2, \tau_n = 4\}, V_4 = V_{3,4} = \{n \in V(R) | d_n = 3, \tau_n = 4\}$ $\tau_n = 4$, $V_5 = V_{3,5} =$ {n \in V (*R*)| $d_n = 3$, $\tau_n = 5$ } and $V_6 = V_{4,8} =$ {n \in V (*R*) $| \mathbf{d}_n = 4, \ \tau_n = 8$, where $| \mathbf{V}_1 | = 8p, \ | \mathbf{V}_2 | = 50p + 1, \ | \mathbf{V}_3 | = 14p, \ | \mathbf{V}_4 | = 22p$ $+1$, $|V_5| = 16p$ and $|V_6| = 4p$, So, $|V(R)| = |V_1| + |V_2| + |V_3| + |V_4| + |V_5|$ V_5 | $|V_6|$ = 114p +2. The partitions of network R vertices are presented in the following Tables 1, 2 and 3.

Table 1. The Partitions of Network R Vertices with the Help of Degree

	THEIR IS THE FULLMOINS OF FIGHTOIN IN TURNOW WHILE THE FIGHT OF DUCTION		
$42p+30$	$26p+14$	$2p+2$	

Table 2. The Partitions of Network R Vertices with the Help of Connection Number

There are four types of partitions having edge sets of *R* with respect to the degree as $|E(R)| = |E_{2,2}^d| + |E_{2,3}^d| + |E_{3,3}^d| + |E_{3,4}^d| = 85p + 55$. There are seven types of partitions having edge sets of *R* with respect to connection number of vertices as $|E(R)| = |E_{2,3}^c| + |E_{3,3}^c| + |E_{3,4}^c| + |E_{3,5}^c| + |E_{4,4}^c| + |E_{4,5}^c|$ $+ |E_{5,8}^c| = 85p + 55$. The partitions of network R edges are presented in the following Tables 4 and 5.

Table 4. The Partitions of Network R Edges with the Help of Degree

$\mathbf{\Gamma}^d$ $L_{d(m),d(n)}$	\mathbf{r} a د دینا \leftharpoonup, \perp	\mathbf{r} d $E_{2,3}$	\mathbf{r} d -3.3	$\mathbf{\Gamma}^d$ $\bm{\nu}_{3,4}$
Γ ^d $\left E_{d(m),d(n)}\right $	$6p+16$	$52p + 28$	$9p+3$	$8p+8$

Table 5. The Partitions of Network R Edges with the Help of Connection Number

Definition 2.8. Zinc Silicate Network (ZNSL(p)): Silicate is one of the most interesting largest class of mineral in the world. $SiO₄$ is a mixture of sand and metal oxide. $SiO₄$ tetrahedron is used as the basic chemical unit of silicate. In graph theory (or chemistry), we represent centre vertices and corner vertices of silicate with silicon nodes (or silicon ions) and oxygen nodes (or oxygen ions), respectively. A silicate sheet is a ring of tetrahedron which is attached to other rings by sharing oxygen nodes with other rings in a two dimensional plane. Such silicate sheets are recognized as sheet-like networks. Some other well-known networks of silicate are pyrosilicate, orthosilicate, chain silicate, cyclic silicate and sheet silicate.

 $Zn_4O(PDC)$ ₃ is also written as IRMOF-14, it is a three dimensional cubic networks having a pore size of $14.7/20.1$ A^0 in diameter, see [\[58\]](#page-25-8). The MON of zinc silicate of dimension 3 is presented in Figure 2.

Figure 2. Zinc silicate network $(ZNSL(p) \cong S)$

Let $S \cong ZNSL(p)$ be the zinc silicate related metal-organic network of dimension p in the plane, see Figure 2. We take partitions of network S with the help of vertex set $V(S)$ and edge set $E(S)$. We see that every vertex has degrees and connection numbers sets as $\{2,3,4\}$ and $\{2,3,4,5,6,8\}$, respectively. We have $V_1 = \{n \in V(S) | d_n = 2\}$, $V_2 = \{n \in V(S) | d_n = 2\}$ $V(S) | d_n = 3$ and $V_3 = \{ n \in V(S) | d_n = 4 \}$, where $|V_1| = 42p + 30$, $|V_2| = 42p + 30$ V_2 | = 38*p* +18 and | V₃| = 2*p* +2. So, | V(S)| = |V₁ |+ | V₂ | + | V₃| = 82*p* +50. The partition of vertices with respect to connection numbers are

 $V_1 = \{ n \in V(S) | \sigma_n = 2 \}, V_2 = \{ n \in V(S) | \sigma_n = 3 \}, V_3 = \{ n \in V(S) \}$ $| \tau_n = 4 \}, V_4 = \{ n \in V(S) | \tau_n = 5 \}, V_5 = \{ n \in V(S) | \tau_n = 6 \}, \text{ and } V_6 = 6 \}.$ { $n \in V(S)$ | $\tau_n = 8$ }, where | V₁| = 2p+6, | V₂| = 16p+16, | V₃| = 48p+16, | V_4 | = 8p+8, | V_5 | = 6p+2 and | V_6 | = 2p+2. So, $|V(S)| = |V_1| + |V_2| + |V_3|$ $+|V_4| + |V_5| + |V_6| = 82p + 50$. Now, the partition of vertices with respect to degrees and connection numbers are

$$
V_1 = V_{d,\tau} = V_{2,2} = \{n \in V(S) | d_n = 2, \tau_n = 2\}, V_2 = V_{2,3} = \{n \in V(S) | d_n = 2, \tau_n = 3\}, V_3 = V_{2,4} = \{n \in V(S) | d_n = 2, \tau_n = 4\}, V_4 = V_{3,4} = \{n \in V(S) | d_n = 2, \tau_n = 4\}
$$

 $|d_n = 3, \tau_n = 4|, V_5 = V_{3,5} = \{n \in V(S) | d_n = 3, \tau_n = 5\}, V_6 = V_{3,6} = \{n \in V_{3,6}\}$ V (S) $| d_n = 3, \tau_n = 6$, and $V_7 = V_{4,8} = {n \in V (S) | d_n = 4, \tau_n = 8}$ where $| V_1 | = 8p, | V_2 | = 30p +1, | V_3 | = 30p +3, | V_4 | = 30p +3, | V_5 | = 14p +1$ and $|V_6| = 8p$ and $|V_7| = 4p$ So, $|V(S)| = |V_1| + |V_2| + |V_3| + |V_4| + |V_5| + |V_5|$ V_6 |+| V_7 | = 124p +8. The partitions of network S vertices are presented in the following Tables 6, 7 and 8.

Table 6. The Partitions of Network S Vertices with the Help of Degree V_d **2 3 4** $|V_{d}|$ $42p+30$ $38p+18$ $2p+2$

Table 7. The Partitions of Network S Vertices with the Help of Connection Number

$V\tau$				
		$ V_r $ 2p+6 16p+16 48p+16 8p+8 6p+2 2p+2		

Table 8. The Partitions of Network S Vertices with the Help of Degree and Connection Number

Now, there are four types of partitions having edge sets of *S* with respect to the degree as $|E(S)| = |E_{2,2}^d| + |E_{2,3}^d| + |E_{3,3}^d| + |E_{3,4}^d| = 103p + 61$. There are seven types of partitions having edge sets of *S* with respect to connection number of vertices as $|E(S)| = |E_{2,3}^c| + |E_{3,3}^c| + |E_{3,4}^c| + |E_{3,5}^c| +$ $|E_{4,4}^c|+|E_{4,5}^c|+|E_{4,6}^c|+|E_{5,8}^c|+|E_{6,6}^c|=103p+61$. The partitions of network S edges are presented in the following Tables 9 and 10.

Table 9. The Partitions of Network S Edges with the Help of Degree

\mathbf{r} d $L_{d(m),d(n)}$	гa ن د شم $\overline{}$	гa -22 د, ک	\mathbf{r} a 3 ج سا د, د	\mathbf{E}^d $L_{3,4}$
$\left E_{d(m),d(n)}^d \right $	$10p+14$	$64p+32$	$21p+7$	$8p+8$

TAMITTOM					
$E^c_{\tau(m),\tau(n)}$	$E^c_{2,3}$	$E_{3,3}^c$	$E_{3,4}^c$	$E_{3,5}^c$	$E_{\rm 4.4}^{c}$
$\left E_{\tau(m),\tau(n)}^c\right $	$4p+12$	$6p+2$	$12p+4$	$4p+12$	$42p+14$
$E^c_{\tau(m),\tau(n)}$	$E_{4,5}^c$	$E_{4,6}^{c}$	$E_{5,8}^c$	$E^c_{6,6}$	
$\left E_{\tau(m),\tau(n)}^c\right $	$12p+4$	$12p+4$	$8p+8$	$3p+1$	

Table 10. The Partitions of Network S Edges with the Help of Connection Number

3. Main Results for MONs

This section computes the main results for the first, second, third, fourth and fifth multiplicative Zagreb connection indices of zinc oxide and zinc silicate related MONs.

Theorem 3.1: Let $R \cong ZNOX(p)$ and $S \cong ZNSL(p)$ be two MONs of dimensions p. Then, the first multiplicative ZCI of two MONs R and S are as follows:

(a)

 $MZC_1(R) = 2.4772608 \times 10^{10} p^5 + 1.49815296 \times 10^{11} p^4 + 3.016359936 \times 10^{11} p^3$ $+ 2.504392704 \times 10^{11} p^2 + 7.56154368 \times 10^{10} p + 1.769472000 \times 10^9$,

(b)

 $MZC_1(S) = 4.892236186 \times 10^{12} p^6 + 3.261490421 \times 10^{13} p^5 + 7.881936078$ $\times 10^{13}$ p^4 +9.132173844 $\times 10^{13}$ p^3 +5.381459805 $\times 10^{13}$ p^2 +1.522029036 $\times 10^{13}$ p $+1.630745795\times10^{12}$

Proof (a). By principle,

$$
MZC_1(K) = \prod_{n \in V(K)} [\tau_K(n)]^2
$$

=
$$
\prod_{n \in V_2^c} [\tau_R(n)]^2 \times \prod_{n \in V_3^c} [\tau_R(n)]^2 \times \prod_{n \in V_4^c} [\tau_R(n)]^2 \times \prod_{n \in V_5^c} [\tau_R(n)]^2 \times \prod_{n \in V_8^c} [\tau_R(n)]^2
$$

By using Table 2,

Ali

$$
= (2p+6)(2)^2 \times (28p+20)(3)^2 \times (30p+10)(4)^2 \times (8p+8)(5)^2 \times (2p+2)(8)^2
$$

= (2016p² + 7488p + 4320) × (96000p² + 128000p + 3200) × (128p+128)
= 2.4772608 × 10¹⁰ p⁵ + 1.49815296 × 10¹¹ p⁴ + 3.016359936 × 10¹¹ p³
+ 2.504392704 × 10¹¹ p² + 7.56154368 × 10¹⁰ p + 1.769472000 × 10⁹.
(b). By principle,

$$
MZC_1(K) = \prod_{n \in V(K)} [\tau_K(n)]^2
$$

 $\prod_{n\in V_2^c}$ $=$ $n \in V_2^c$ $[\tau_S(n)]^2 \times \prod_{n \in V_S^c}$ $[\tau_S(n)]^2 \times \prod_{n \in V_4^c}$ $[\tau_{S}(n)]^{2} \times \prod_{n \in V_{S}^{c}}$ $[\tau_{S}(n)]^{2} \times \prod_{n \in V_{6}^{c}}$ $[\tau_s(n)]^2 \times$ $\prod_{n\in V^c_8}$ $[\tau_{S}(n)]^{2}$

By using Table 7,

$$
= (2P+6)(2)^2 \times (16p+16)(3)^2 \times (48p+16)(4)^2 \times (8p+8)(5)^2 \times (6p+2)(6)^2 \times
$$

\n
$$
(2p+2)(8)^2
$$

\n
$$
= (1152p^2 + 4608p + 3456) \times (153600p^2 + 204800p + 51200) \times (27648p^2 + 36864p + 9216)
$$

\n
$$
= 4.892236186 \times 10^{12}p^6 + 3.261490421 \times 10^{13}p^5 + 7.881936078 \times 10^{13}p^4 + 9.132173844 \times 10^{13}p^3 + 5.381459805 \times 10^{13}p^2 + 1.522029036 \times 10^{13}p + 1.630745795 \times 10^{12}.
$$

Theorem 3.2: Let $R \cong ZNOX(p)$ and $S \cong ZNSL(p)$ be two MONs of dimensions p. Then, the second multiplicative ZCI of two MONs R and S are as follows:

(a)

$$
MZC_2(R) = 9.57655233 \times 10^{14} p^8 + 1.33829567 \times 10^{17} p^7 + 9.785365205 \times 10^{17} p^6 + 2.469533816 \times 10^{18} p^5 + 2.48995058 \times 10^{18} p^4 + 11.43990477 \times 10^{17} p^3
$$

+ 2.729399844 × 10¹⁷ p² + 4.004443423 × 10¹⁶ p + 3.522410054 × 10¹⁵,

(b)

 $MZC_2(S) = 1.479074071 \times 10^{21} p^{10} + 1.380469133 \times 10^{22} p^9 + 4.979549374 \times$ 10^{22} p^8 + 9.11547872 × 10^{22} p^7 + 9.688848174 × 10^{22} p^6 + 6.931561944 × 10^{22} $p^5 + 2.775140623 \times 10^{22} p^4 + 13.68160423 \times 10^{22} p^2 + 13.7965757 \times 10^{19} p +$ 6.086724573×10^{18} .

Proof (a). By principle,

$$
MZC_{2}(K) = \prod_{mn \in E(K)} [\tau_{K}(m) \times \tau_{K}(n)]
$$

\n
$$
= \prod_{mn \in E_{2,3}^{c}} [\tau_{R}(m) \times \tau_{R}(n)] \times \prod_{mn \in E_{3,3}^{c}} [\tau_{R}(m) \times \tau_{R}(n)] \times \prod_{mn \in E_{3,5}^{c}} [\tau_{R}(m) \times \tau_{R}(n)] \times
$$

\n
$$
\prod_{mn \in E_{4,4}^{c}} [\tau_{R}(m) \times \tau_{R}(n)]
$$

\n
$$
\times \prod_{mn \in E_{4,4}^{c}} [\tau_{R}(m) \times \tau_{R}(n)] \times \prod_{mn \in E_{3,4}^{c}} [\tau_{R}(m) \times \tau_{R}(n)] \times \prod_{mn \in E_{4,4}^{c}} [\tau_{R}(m) \times \tau_{R}(n)] \times
$$

\n
$$
\prod_{mn \in E_{5,8}^{c}} [\tau_{R}(m) \times \tau_{R}(n)]
$$

\n
$$
= \left| E_{2,3(R)}^{c} \right| (2)(3) \times \left| E_{3,3(R)}^{c} \right| (3)(3) \times \left| E_{3,5(R)}^{c} \right| (3)(5) \times \left| E_{4,5(R)}^{c} \right| (4)(5) \times \left| E_{4,4(R)}^{c} \right|
$$

 $(4)(4) \times \left| E_{3,4(R)}^c \right| (3)(4) \times \left| E_{4,4(R)}^c \right| (4)(4) \times \left| E_{5,8(R)}^c \right| (5)(8)$

By using Table 5,

 $=(4p+12)(6)\times(12p+4)(9)\times(4p+12)(15)\times(12p+4)(20)\times(12p+4)(16)\times$ $(24p+8)(12)\times(9p+3)(16)\times(8p+8)(40)$ $= (2592 p² + 8640 p + 2592) \times (14400 p² + 48000 p + 14400) \times (55296 p² +$ $36864 p + 6144 \times (464 p^2 + 61440 p + 15360)$ $= 9.57655233 \times 10^{14} p^8 + 1.33829567 \times 10^{17} p^7 + 9.785365205 \times 10^{17} p^6 +$ $2.469533816\times10^{18} p^5 + 2.48995058\times10^{18} p^4 + 11.43990477\times10^{17} p^3 +$ $2.729399844 \times 10^{17} p^2 + 4.004443423 \times 10^{16} p + 3.522410054 \times 10^{15}$.

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(b). By principle, $\prod_{v\in E\left(.\right) }% \sum_{v\in E\left(.\right) }\left\vert 1_{v}\right\vert ^{2}$ $=$ (K) $_{2}(K)$ $mn \in E(K)$ $MZC_2(K) = \prod \left[\tau_K(m) \times \tau_K(n) \right]$ $\prod_{n\in E_2^c}$ $=$ $mn \in E_{2,3}^c$ $[\tau_S(m) \times \tau_S(n)] \times \prod_{mn \in E_{3,3}^c}$ $[\tau_S(m) \times \tau_S(n)] \times \prod_{mn \in E_{3,5}^c}$ $[\tau_s(m) \times \tau_s(n)] \times$ $\prod_{mn\in E_{4,5}^c}$ $[\tau_s(m) \times \tau_s(n)]$ \times $\prod_{mn\in E_{4,4}^c}$ $[\tau_S(m) \times \tau_S(n)] \times \prod_{mn \in E_{3,4}^c}$ $[\tau_S(m) \times \tau_S(n)] \times \prod_{mn \in E_{4,4}^c}$ $[\tau_{S}(m) \times \tau_{S}(n)] \times$ $\prod_{mn\in E_{4,6}^c}$ $[\tau_S(m) \times \tau_S(n)] \times \prod_{mn \in E_{6,6}^c}$ $[\tau_S(m) \times \tau_S(n)] \times \prod_{mn \in E_{5,8}^c}$ $[\tau_{s}(m) \times \tau_{s}(n)]$ $E_{2,3(S)}^{c} | (2)(3) \times |E_{3,3(S)}^{c} | (3)(3) \times |E_{3,5(S)}^{c} | (3)(5) \times |E_{4,5(S)}^{c} | (4)(5) \times |E_{4,4(S)}^{c} |$ $(4)(4) \times \left| E_{3,4(S)}^c \right|$ $(3)(4) \times \left| E_{4,4(S)}^c \right|$ $(4)(4) \times \left| E_{4,6(S)}^c \right|$ $(4)(6) \times \left| E_{6,6(S)}^c \right|$ $(6)(6) \times$ $E_{5,8(S)}^{c}$ (5)(8) By using Table 10, $=(4p+12)(6)\times(6p+2)(9)\times(4p+12)(15)\times(12p+4)(20)\times(36p+12)(16)\times$ $(12p+4)(12)\times(6p+2)(16)\times(12p+4)(24)\times(3p+1)(36)\times(8p+8)(40)$ $=$ (1296 p^2 + 4320 p + 1296) \times (14400 p^2 + 48000 p + 14400) \times (82944 p^2 +

 $55296p + 9216 \times (27648p^2 + 18432p + 3072) \times (34560p^2 + 46080p + 11520)$ $= 1.479074071 \times 10^{21} p^{10} + 1.380469133 \times 10^{22} p^{9} + 4.979549374 \times 10^{22} p^{8} +$ $29.688848174 \times 10^{22} p^6 + 6.931561944 \times 10^{22} p^5 + 2.775140623 \times 10^{22} p^4 +$ p 7.769365766 \times 10 21 p^{3} +13.68160423 \times 10 22 p^{2} +13.7965757 \times 10 19 p + $6.086724573\times 10^{18}$.

Theorem 3.3: Let $R \cong ZNOX(p)$ and $S \cong ZNSL(p)$ be two MONs of dimensions p. Then, the third multiplicative ZCI of two MONs R and S are as follows:

(a)

 $MZC₂(R) = 8.719958016 \times 10^{12} p^6 + 5.707608883 \times 10^{11} p^5 + 7.927234560$ $\times 10^{9} p^{4},$

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(b)

 $MZC_3(S) = 1.926317998 \times 10^{15} p^7 + 5.872683423 \times 10^{14} p^6 + 6.421059994$ $\times 10^{13} p^5 + 2.935341711 \times 10^{12} p^4 + 4.586471424 \times 10^{10} p^3$.

Proof (a). By principle,

$$
MZC_{3}(K) = \prod_{n \in V(K)} [d_{K}(n) \times \tau_{K}(n)]
$$

=
$$
\prod_{n \in V_{2,2}} [d_{R}(n) \times \tau_{R}(n)] \times \prod_{n \in V_{2,3}} [d_{R}(n) \times \tau_{R}(n)] \times \prod_{n \in V_{2,4}} [d_{R}(n) \times \tau_{R}(n)] \times \prod_{n \in V_{3,4}} [d_{R}(n) \times \tau_{R}(n)]
$$

$$
\times \prod_{n \in V_{3,5}} [d_{R}(n) \times \tau_{R}(n)] \times \prod_{n \in V_{4,8}} [d_{R}(n) \times \tau_{R}(n)]
$$

By using Table 3,

$$
= (8p)(2 \times 2) \times (50p + 1)(2 \times 3) \times (14p)(2 \times 4) \times (22p + 1)(3 \times 4) \times (16p)(3 \times 5)
$$

×(4p)(4×8)

 $p^2 + 192p \times (29568p^2 + 1344p) \times (30720p^2)$

 $= 8.719958016 \times 10^{12} p^{6} + 5.707608883 \times 10^{11} p^{5} + 7.927234560 \times 10^{9} p^{4}$.

(b). By principle,

$$
MZC_{3}(K) = \prod_{n \in V(K)} [d_{K}(n) \times \tau_{K}(n)]
$$

\n
$$
= \prod_{n \in V_{2,2}} [d_{S}(n) \times \tau_{S}(n)] \times \prod_{n \in V_{2,3}} [d_{S}(n) \times \tau_{S}(n)] \times \prod_{n \in V_{2,4}} [d_{S}(n) \times \tau_{S}(n)] \times \prod_{n \in V_{3,4}} [d_{S}(n) \times \tau_{S}(n)]
$$

\n
$$
\times \prod_{n \in V_{3,5}} [d_{S}(n) \times \tau_{S}(n)] \times \prod_{n \in V_{3,6}} [d_{S}(n) \times \tau_{S}(n)] \times \prod_{n \in V_{4,8}} [d_{S}(n) \times \tau_{S}(n)]
$$

\nBy using Table 8,
\n
$$
= (8p)(2 \times 2) \times (30p + 1)(2 \times 3) \times (30p + 3)(2 \times 4) \times (30p + 3)(3 \times 4) \times (14p + 1)
$$

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 $(3\times5)\times(8p)(3\times6)\times(4p)(4\times8)$

 $= (5760p^2 + 192p) \times (86400p^2 + 17280p + 864) \times (30240p^2 + 2160p) \times (128p^2)$ $= 1.926317998 \times 10^{15} p^7 + 5.872683423 \times 10^{14} p^6 + 6.421059994 \times 10^{13} p^5 + 2.935341711$ $\times 10^{12} p^4 + 4.586471424 \times 10^{10} p^3$.

Theorem 3.4: Let $R \cong ZNOX(p)$ and $S \cong ZNSL(p)$ be two MONs of dimensions p. Then, the fourth multiplicative ZCI of two MONs R and S are as follows:

$$
(a)
$$

 $MZC_4(R) = 6.010112154 \times 10^{14} p^8 + 5.208763867 \times 10^{15} p^7 + 16.69475598 \times$ $10^{15} p^6 + 2.533150975 \times 10^{16} p^5 + 2.062710329 \times 10^{16} p^4 + 9.611232853 \times 10^{15}$ $p^3 + 2.577175665 \times 10^{15} p^2 + 3.709945774 \times 10^{14} p + 2.225967464 \times 10^{13}$

(b)

$$
MZC_4(S) = 1.298184225 \times 10^{18} p^{10} + 1.21163861 \times 10^{19} p^9 + 4.370553558 \times 10^{19} p^8 + 3.915708269 \times 10^{19} p^7 + 8.503908024 \times 10^{19} p^6 + 5.6457658 \times 10^{19} p^5
$$

+ 2.383565961 \times 10^{19} p^4 + 5.69847671 \times 10^{18} p^3 6.309875773 \times 10^{17} p^2 +
3.561547944 \times 10^{16} p + 5.342321915 \times 10^{15}.

Proof (a). By principle,

$$
= (5760p^2 + 192p) \times (86400p^2 + 17280p + 864) \times (30240p^2 + 2160p) \times (128p)
$$

\n
$$
= 1.926317998 \times 10^{15} p^7 + 5.872683423 \times 10^{14} p^6 + 6.421059994 \times 10^{13} p^5 + 2.935341711
$$

\n
$$
\times 10^{12} p^4 + 4.586471424 \times 10^{10} p^3.
$$

\n**Theorem 3.4:** Let $R \approx \mathbb{ZNOX}(p)$ and $S \approx \mathbb{ZNSL}(p)$ be two MONs of dimensions p. Then, the fourth multiplicative ZCI of two MONs R and S are as follows:
\n(a)
\n
$$
MZC_4(R) = 6.010112154 \times 10^{14} p^8 + 5.208763867 \times 10^{15} p^7 + 16.69475598 \times 10^{15} p^6 + 2.533150975 \times 10^{16} p^5 + 2.062710329 \times 10^{16} p^4 + 9.611232853 \times 10^{15} p^3 + 2.577175665 \times 10^{15} p^2 + 3.709945774 \times 10^{14} p + 2.225967464 \times 10^{13},
$$

\n
$$
p^3 + 2.577175665 \times 10^{15} p^2 + 3.709945774 \times 10^{14} p + 2.225967464 \times 10^{13},
$$

\n
$$
p^8 + 3.915708269 \times 10^{19} p^7 + 8.503908024 \times 10^{19} p^6 + 5.6457658 \times 10^{19} p^5
$$

\n
$$
+ 2.383565961 \times 10^{19} p^4 + 5.69847671 \times
$$

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$$
= \left| E_{2,3(R)}^c \right| (2+3) \times \left| E_{3,3(R)}^c \right| (3+3) \times \left| E_{3,5(R)}^c \right| (3+5) \times \left| E_{4,5(R)}^c \right| (4+5) \times \left| E_{4,4(R)}^c \right|
$$

$$
(4+4) \times \left| E_{3,4(R)}^c \right| (3+4) \times \left| E_{4,4(R)}^{c^*} \right| (4+4) \times \left| E_{5,8(R)}^c \right| (5+8)
$$

By using Table 5,

$$
= (4p+12)(5) \times (12p+4)(6) \times (4p+12)(8) \times (12p+4)(9) \times (12p+4)(8) \times (24p+8)(7) \times (9p+3)(8) \times (8p+8)(13)
$$

$$
= (1440p2 + 4800p + 1440)(3456p2 + 11520p + 3456)(16128p2 + 10752p
$$

+ 1792)(7488p² + 9984p + 2496)

 $= 6.010112154 \times 10^{14} p^8 + 5.208763867 \times 10^{15} p^7 + 16.69475598 \times 10^{15} p^6 +$ $12.533150975 \times 10^{16} p^5 + 2.062710329 \times 10^{16} p^4 + 9.611232853 \times 10^{15} p^3 +$ $2.577175665\times10^{15} p^2 + 3.709945774\times10^{14} p + 2.225967464\times10^{13}$.

(b). By principle,

$$
MZC_{4}(K) = \prod_{mneE(K)} [\tau_{K}(m) + \tau_{K}(n)]
$$

\n
$$
= \prod_{mneE_{2,3}^{c}} [\tau_{S}(m) + \tau_{S}(n)] \times \prod_{mneE_{3,3}^{c}} [\tau_{S}(m) + \tau_{S}(n)] \times \prod_{mneE_{3,5}^{c}} [\tau_{S}(m) + \tau_{S}(n)] \times
$$

\n
$$
\prod_{mneE_{4,5}^{c}} [\tau_{S}(m) + \tau_{S}(n)] \times \prod_{mneE_{4,4}^{c}} [\tau_{S}(m) + \tau_{S}(n)] \times \prod_{mneE_{3,4}^{c}} [\tau_{S}(m) + \tau_{S}(n)] \times \prod_{mneE_{4,4}^{c}} [\tau_{S}(m) + \tau_{S}(n)]
$$

\n
$$
\times \prod_{mneE_{4,6}^{c}} [\tau_{S}(m) + \tau_{S}(n)] \times \prod_{mneE_{6,6}^{c}} [\tau_{S}(m) + \tau_{S}(n)] \times \prod_{mneE_{5,8}^{c}} [\tau_{S}(m) + \tau_{S}(n)]
$$

\n
$$
= |E_{2,3(S)}^{c}| (2+3) \times |E_{3,3(S)}^{c}| (3+3) \times |E_{3,5(S)}^{c}| (3+5) \times |E_{4,5(S)}^{c}| (4+5) \times |E_{4,4(S)}^{c}| (4+4) \times |E_{3,8(S)}^{c}| (5+8)
$$

By using Table 10,

$$
= (4p+12)(5) \times (6p+2)(6) \times (4p+12)(8) \times (12p+4)(9) \times (36p+12)(8) \times
$$

(12p+4)(7) \times (6p+2)(8) \times (12p+4)(10) \times (3p+1)(12) \times (8p+8)(13)

$$
= (720p^2 + 2400p + 720) \times (3456p^2 + 11520p + 3456) \times (24192p^2 +
$$

16128p+2688) \times (5760p^2 + 3840p + 640) \times (3744p^2 + 4992p + 1248)

$$
= 1.298184225 \times 10^{18} p^{10} + 1.21163861 \times 10^{19} p^9 + 4.370553558 \times 10^{19} p^8 +
$$

3.915708269 \times 10^{19} p^7 + 8.503908024 \times 10^{19} p^6 + 5.6457658 \times 10^{19} p^5 +
2.383565961 \times 10^{19} p^4 + 5.69847671 \times 10^{18} p^3 6.309875773 \times 10^{17} p^2 +
3.561547944 \times 10^{16} p + 5.342321915 \times 10^{15}.

Theorem 3.5: Let $R \cong ZNOX(p)$ and $S \cong ZNSL(p)$ be two MONs of dimensions p. Then, the fifth multiplicative ZCI of two MONs R and S are as follows:

(a)

 $=$

 $n \in V_{3,5}$

 $MZC_5(R) = 6.35830272 \times 10^{11} p^6 + 4.161798144 \times 10^{10} p^5 + 5.78027520 \times 10^8 p^4$, **(b)**

 $MZC_5(S) = 7.023034368 \times 10^{13} p^7 + 2.140353331 \times 10^{13} p^6 + 2.341011456 \times$ $10^{12} p^5 + 1.070176666 \times 10^{11} p^4 + 1.672151040 \times 10^9 p^3$.

Proof (a). By principle,

$$
MZC_{5}(K) = \prod_{n \in V(K)} [d_{K}(n) + \tau_{K}(n)]
$$

=
$$
\prod_{n \in V_{2,2}} [d_{R}(n) + \tau_{R}(n)] \times \prod_{n \in V_{2,3}} [d_{R}(n) + \tau_{R}(n)] \times \prod_{n \in V_{3,4}} [d_{R}(n) + \tau_{R}(n)] \times \prod_{n \in V_{3,4}} [d_{R}(n) + \tau_{R}(n)]
$$

$$
\times \prod [d_{R}(n) + \tau_{R}(n)] \times \prod [d_{R}(n) + \tau_{R}(n)]
$$

By using Table 3,

$$
=(8p)(2+2)\times(50p+1)(2+3)\times(14p)(2+4)\times(22p+1)(3+4)\times(16p)
$$

(3+5)\times(4p)(4+8)

 $n \in V_{4,8}$

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 $n \in V_{3,4}$

$$
= (8000p2 + 160p) \times (12936p2 + 588p) \times (6144p2)
$$

= 6.35830272×10¹¹ p⁶ + 4.161798144×10¹⁰ p⁵ + 5.78027520×10⁸ p⁴.
(**b**). By principle,

$$
MZC_{5}(K) = \prod_{n \in V(K)} [d_{K}(n) + \tau_{K}(n)]
$$

\n
$$
= \prod_{n \in V_{2,2}} [d_{S}(n) + \tau_{S}(n)] \times \prod_{n \in V_{2,3}} [d_{S}(n) + \tau_{S}(n)] \times \prod_{n \in V_{2,4}} [d_{S}(n) + \tau_{S}(n)] \times \prod_{n \in V_{3,4}} [d_{S}(n) + \tau_{S}(n)]
$$

\n
$$
\times \prod_{n \in V_{3,5}} [d_{S}(n) + \tau_{S}(n)] \times \prod_{n \in V_{3,6}} [d_{S}(n) + \tau_{S}(n)] \times \prod_{n \in V_{4,8}} [d_{S}(n) + \tau_{S}(n)]
$$

By using Table 8,

$$
= (8p)(2+2) \times (30p+1)(2+3) \times (30p+3)(2+4) \times (30p+3)(3+4) \times (14p+1)(3+5) \times (8p)(3+6) \times (4p)(4+8)
$$

$$
= (4800p2 + 160p) \times (37800p2 + 7560p + 3787) \times (387072p3 + 27648p2)
$$

= 7.023034368×10¹³ p⁷ + 2.140353331×10¹³ p⁶ + 2.341011456×10¹² p⁵
+ 1.070176666×10¹¹ p⁴ + 1.672151040×10⁹ p³.

4. Conclusion

In this paper, we computed the first, second, third, fourth and fifth multiplicative Zagreb connection indices of two different zinc oxide (R) and zinc silicate (S) related MONs by keeping in mind the increasing layer p for both metal ions and organic linkers.

Future researchers can compute the multiplicative Zagreb connection indices (ZCIs) of other MONs with respect to the degree and connection number-based TIs. Further research can also be done on other MONs using Randic index, general Randic index, general first Zagreb index, and modified multiplicative Zagreb connection indices.

Conflict of Interest

The author declare no conflict of interest.

References

- [1] Cui Y, Xu H, Yue Y, et al. A luminescent mixed-lauthanide metalorganic framework thermometer. *J Am Chem Soc.* 2012;134:3979- 3982. <https://doi.org/10.1021/ja2108036>
- [2] Wang C, Tian L, Zhu W, et al. Dye@bio-MOF-1 composite as a dual emitting platform for explosive molecules. *ACS Appl Mater Interfaces,* 2017;9:20076-20085. <https://doi.org/10.1021/acsami.7b04172>
- [3] Bahrani S, Hashemi SA, Mousavi SM, Azhdari R. Zinc-based metalorganic frameworks as nontoxic and biodegradable platforms for biomedical applications: review study. *Drug Metabolism Rev*. 2019;51(3):356-377. <https://doi.org/10.1080/03602532.2019.1632887>
- [4] Eddaoudi M, Kim J, Rosi N, et al. Systematic design of pore size and functionality in isoreticular MOFs and their application in methane storage. *Sci.* 2002;295:469-472. https://doi.org[/10.1126/science.1067208](https://doi.org/10.1126/science.1067208)
- [5] Keskin S, Sholl D. Efficient methods for screening of metal organic frame work membranes for gas separations using atomically detailed models. *Langmuir.* 2009;25(19):11786-11795.
- [6] Ahmad I, Jhung SH. Composites of metal-organic frameworks: preparation and application in adsorption. *Mater Today,* 2014;17(3):136-146. <https://doi.org/10.1016/j.mattod.2014.03.002>
- [7] Li H, Li L, Lin R.-B, et al. Porous metal-organic frameworks for gas storage and separation: status and challenges. *EnergyChem.* 2019;1(1):100006.<https://doi.org/10.1016/j.enchem.2019.100006>
- [8] Thornton AW, Nairn KM, Hill JM, Hill AJ, Hill MR. Metal-organic frameworks impregnated with magnesium-decorated fullerenes for methane and hydrogen storage. *J Am Chem Soc.* 2009;131(30):10662- 10669. <https://doi.org/10.1021/ja9036302>
- [9] Hwang YK, Hong DY, Chang JS, Jhung SH, Seo YK, Kim J. Amine grafting on coordinatively unsaturated metal centers of MOFs: consequences for catalysis and metal encapsulation. *Angew Chem Int Edit.* 2008;47(22):4144-4148.<https://doi.org/10.1002/ange.200705998>
- [10] Ding G, Yuan J, Jin F, et al. High performance all-polymer nonfullerence solar cells by employing an efficient polymer-small molecule acceptor alloy strategy. *Nano Energy.* 2017;36:356-365. <https://doi.org/10.1016/j.nanoen.2017.04.061>
- [11] Yin Z, Zhou YL, Zeng MH, Kurmoo M. The concept of mixed organic ligands in metal–organic frameworks: design, tuning and functions. *Dalton T.* 2015;44(12):5258-5275. [https://doi.org/10.1039/](https://doi.org/10.1039/%20C4DT04030A) [C4DT04030A](https://doi.org/10.1039/%20C4DT04030A)
- [12] Kim M, Cahill JF, Fei H, Prather KA, Cohen SM. Postsynthetic ligand and cation exchange in robust metal–organic frameworks. *J Am Chem Soc.* 2012;134(43):18082-18088. [https://doi.org/10.1021/](https://doi.org/10.1021/%20ja3079219) [ja3079219](https://doi.org/10.1021/%20ja3079219)
- [13] Lin RB, Xiang S, Xing H, Zhou W, Chen B. Exploration of porous metal–organic frameworks for gas separation and purification. *Coordin Chem Rev.* 2019;378:87-103. [https://doi.org/10.1016/](https://doi.org/10.1016/%20j.ccr.2017.09.027) [j.ccr.2017.09.027](https://doi.org/10.1016/%20j.ccr.2017.09.027)
- [14] Mandal B, Chung JS, Kang SG. Exploring the geometric, magnetic and electronic properties of Hofmann MOFs for drug delivery. *Phys Chem Chem Phys*. 2017;19(46):31316-31324. [https://doi.org/](https://doi.org/%2010.1039/C7CP04831A) [10.1039/C7CP04831A](https://doi.org/%2010.1039/C7CP04831A)
- [15] Geier SJ, Mason JA, Bloch ED. Selective adsorption of ethylene over ethane and propylene over propane in the metal-organic frameworks M2 (dobdc) (M=Mg, Mn, Fe, Co, Ni, Zn). *Chem Sci.* 2013;4(5):2054–2061. <https://doi.org/10.1039/C3SC00032J>
- [16] Murray LJ, Dinca M, Long JR. Hydrogen storage in metal-organic frameworks. *Chem Soc Rev.* 2009;38(5);1294–1314. [https://doi.org/](https://doi.org/%2010.1039/B802256A) [10.1039/B802256A](https://doi.org/%2010.1039/B802256A)
- [17] Rosi NL, Eckert J, Eddaoudi M. Hydrogen storage in microporous metal-organic frameworks. *Sci.* 2003;300(5622):1127–1129.
- [18] Kennedy RD, Krungleviciute V, Clingerman DJ. Carborane-based metal-organic framework with high methane and hydrogen storage capacities. *Chem Mater.* 2013;25(17):3539–3543. [https://doi.org/](https://doi.org/%2010.1021/cm4020942) [10.1021/cm4020942](https://doi.org/%2010.1021/cm4020942)

- [19] Sarkisov L. Toward rational design of metal-organic frameworks for sensing applications: efficient calculation of adsorption characteristics in zero loading regime. *J Phys Chem C.* 2012;116(4):3025–3033. <https://doi.org/10.1021/jp210633w>
- [20] Li J.-R, Kuppler RJ, Zhou H.-C. Selective gas adsorption and separation in metal-organic frameworks. *Chem Soc Rev.* 2009;38(5):1477–1504. <https://doi.org/10.1039/B802426J>
- [21] Kim JY, Balderas-Xicohtencatl R, Zhang L. Exploiting diffusion barrier and chemical affinity of metalorganic frameworks for efficient hydrogen isotope separation. *J Am Chem Soc.* 2017;139(42)15135– 15141.
- [22] Klavzar S, Gutman I. Selected properties of the Schultz molecular topological index. *J Chem Inf Comput Sci*. 1996;36:1001-1003. <https://doi.org/10.1021/ci9603689>
- [23] Rucker G, Rucker C. On topological indices, boiling points and cycloalkanes. *J Chem Inf Comp Sci.* 1999;39:788-802. <https://doi.org/10.1021/ci9900175>
- [24] Gonzalez-Diaz H, Vilar S, Santana L, Uriarte E. Medicinal chemistry and bioinformatics-current trends in drug discovery with network topological indices. *Cur Top Med Chem.* 2007;7(10):1015-1029.
- [25] Gutman I, Trinajstić N. Graph theory and molecular orbitals. Total π electron energy of alternant hydrocarbons. *Chem Phys Lett.* 1972;17(4):535-538.
- [26] Awais HM, Jamal M, Javaid M. Topological properties of metalorganic frameworks. *Main Group Metal Chem,* 2020;43(1):67-76.
- [27] Hong G, Gu Z, Javaid M, Awais HM, Siddiqui MK. Degree-based topological invariants of metal-organic networks. *IEEE Access,* 2020;8:68288-68300.
- [28] Nadeem MF, Imran M, Siddiqui HMA, Azeem M, Khalil A, Ali Y. Topological aspects of metal-organic structure with the help of underlying networks. *Arabian J Chem.* 2021;14:103157. <https://doi.org/10.1016/j.arabjc.2021.103157>

- [29] Haoer RS. Topological indices of metal-organic networks via neighborhood M-polynomial. *J Discrete Math Sci Cryptography*. 2021;24(2):369-390. <https://doi.org/10.1080/09720529.2021.1888433>
- [30] Kashif A, Aftab S, Javaid M, Awais HM. M-polynomial-based topological indices of metal-organic networks. *Main Group Metal Chem*. 2021;44:129-140.
- [31] Min HY, Kam LF, George ZC. Study suggests choice between green energy or economic growth. *Green Energy Environ.* 2017;2 (8):218– 245.
- [32] Tea KW, Shaopeng Q, Alan FO, Gaurav J, Soo JJ, Vivian TC, Doo KL, Reginald M. Composite nanowires for fast responding and transparent hydrogen sensors. *Am Chem Soc Appl Matter Interf.* 2017;9(45):39464–39474.
- [33] Wasson, MC, Lyu J, Islamoglu T, Farha OK. Linker competition within a metal-organic framework for topological insights. *Inorg Chem.* 2019;58(2):1513–1517. [https://doi.org/10.1021/acs.inorgchem.](https://doi.org/10.1021/acs.inorgchem.%208b03025) [8b03025](https://doi.org/10.1021/acs.inorgchem.%208b03025)
- [34] Tang J.-H, Ali U, Javaid M, Shabbir K. Zagreb connection indices of subdivision and semi-total point operations on graphs. *J Chem.* 2020;9846913:1-14. <https://doi.org/10.1155/2019/9846913>
- [35] Javaid M, Abbas M, Liu J.-B, The WC, Cao J. Topological properties of four-layered neural networks. *JAISCR,* 2019;9(2):111-122.
- [36] Javaid M, Rehman MU, Cao J. Topological indices of rhombus type silicate and oxide networks. *Canadian J Chem*. 2017;95(2):134-43. <https://doi.org/10.1139/cjc-2016-0486>
- [37] Liu J.-B, Raza Z, Javaid M. Zagreb connection indices for cellular neural networks. *Discrete Dyn Nat Soc.* 2020;8038304:1-8.
- [38] Javaid M, Jung CY. M-polynomial and topological indices of silicate and oxide networks. *Int J Pure Appl Math.* 2017;115(1):129-152. <https://doi.org/10.1139/cjc-2016-0486>

- [39] Raheem A, Javaid M, The WC, Wang S, Liu J.-B. M-polynomial method for topological indices of 2D-lattice of three-layered singlewalled titania nanotubes. *J Info Optimization Sci*. 2019;1-11.
- [40] Zhao D, Chu Y.-M, Siddiqui MK, et al. On reverse degree based topological indices of polycyclic metal organic network. *Polycyclic Aromatic Compounds,* 2021. [https://doi.org/10.1080/](https://doi.org/10.1080/%2010406638.2021.1891105) [10406638.2021.1891105](https://doi.org/10.1080/%2010406638.2021.1891105)
- [41] Dayan F, Javaid M, ur Rehman MA. On leap Gourava indices of some wheel related graphs. *Sci Inquiry Rev.* 2018;3(4):13-22. <https://doi.org/10.32350/sir.24.02>
- [42] Dayan F, Javaid M, ur Rehman MA. On leap reduced reciprocal randic and leap reduced second Zagreb indices of some graphs. *Sci Inquiry Rev.* 2019;3(2):27–35.
- [43] Cao J, Ali U, Javaid M, Huang C. Zagreb connection indices of molecular graphs based on opoerations. *Complexity*. 2020;7385682:1- 15.
- [44] Ali U, Javaid M, and Alanazi AM. Computing analysis of connection-based indices and coindices for product of molecular networks. *Symmetry,* 2020;12(8):1320. [https://doi.org/10.3390/sym](https://doi.org/10.3390/sym%2012081320) [12081320](https://doi.org/10.3390/sym%2012081320)
- [45] Ali U, Javaid M. Upper bounds of Zagreb connection indices of tensor and strong product on graphs. *Punjab Uni J Math.* 2020;52(4):89-100.
- [46] Ali U, Javaid M. Zagreb connection indices of disjunction and symmetric difference operations on graphs. *J Prime Res Math.* 2020;16(2):1-15.
- [47] Javaid M, Ali U, Liu J.-B. Computing first Zagreb connection index and coindex of resultant graphs. *Math Prob Eng.* 2021;6019517:1-19.
- [48] Gutman I, Polansky OE. *Mathematical Concepts in Organic Chemistry*. Springer-Verlag Berlin, Heidelberg New York, London, Paris, Tokyo, 1986; DOI: 10.1007/978-3-642-70982-1.
- [49] Todeschini R, Consonni V. *Handbook of molecular descriptors*. John Wiley & Sons;2008.
- [50] Gutman I, Ruscic B, Trinajstić N, Wilson CF. Graph theory and molecular XII. orbitals. Acyclic polyenes. *J Chem Phys.* 1975;62:3399-3405. <https://doi.org/10.1063/1.430994>
- [51] Furtula B, Gutman I. Aforgotten topological index. *J Math Chem.* 2015;53(4):1184-1190.
- [52] Gutman I. Selected properties of the schultz molecular topological index. *J Chem Inf Model.* 1994;34(5):1087-1089. [https://doi.org/](https://doi.org/%2010.1021/ci00021a009) [10.1021/ci00021a009](https://doi.org/%2010.1021/ci00021a009)
- [53] Matamala AR, Estrada E. Generalised topological indices: Optimisation methodology and physico-chemical interpretation. *Chem Phys Lett.* 2005;410(4-6):343_347. [https://doi.org/](https://doi.org/%2010.1016/j.cplett.2005.05.096) [10.1016/j.cplett.2005.05.096](https://doi.org/%2010.1016/j.cplett.2005.05.096)
- [54] Todeschini R, Consonni V. New local vertex invariants and molecular descriptors based on functions of the vertex degrees. *MATCH-Commun Math Comp Chem*. 2010;64:359-372.
- [55] Eliasi M, Gutman I, Iranmanesh A. Multiplicative versions of first Zagreb index. *MATCH Commun Math Comp Chem*. 2012;68:217- 230.
- [56] Ali A, Trinajstić N. A novel/old modification of the first Zagreb index, *Mol Inform.* 2018;37:1-7. <https://doi.org/10.1002/minf.201800008>
- [57] Haoer, RS, Mohammed MA, Selvarasan T, Chidambaram N, Devadoss N. Multiplicative Leap Zagreb Indices of T-thorny Graphs. *Eurasian Chem Commun*. 2020;8:841-846.
- [58] Keskin S, Sholl DS. Screening metal-organic framework materials for membrane-based methane/carbon dioxide seprations. *J Phys Chem.* 2007;111(38):14055-14059. <https://doi.org/10.1021/jp075290l>

